

	$\beta$ - $\alpha$	$\beta$ - $\alpha$	$\gamma$ - $\beta$	$\alpha$ - $\gamma$	$\alpha$ - $\beta$
Avg Number / Frame <sup>1</sup>	0.6	1.1	0.8	0.9	0
Most Frequent <sup>2</sup>	$\alpha$ M1 I228 (40%)/ $\beta$ M2 S265 (40%)	$\beta$ M3 D282 (60%)	$\gamma$ M2 R284 (90%)	$\alpha$ M3 Q287 (70%)	-
Second Most Frequent <sup>2</sup>	$\beta$ M2 T262 (10%)	$\alpha$ M1 Q229 (20%)	$\gamma$ M2 S280 (5%)	$\gamma$ M1 I238 (30%)	-

<sup>1</sup> Number of hydrogen bonds per frame formed between T3 and protein residues lining the cavity, averaged over the second 100 ns of the simulation; values greater than one indicate multiple hydrogen bonds formed in most frames.

<sup>2</sup> Number in parentheses indicates the percentage of the average number/frame that was contributed by this interaction.